3,4-Dihydroxyacetophenone 1197-09-7 | DTXSID30152546

Model Performance

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Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.46

Global applicability domain: Inside

Local applicability domain index: 5.46e-01

Confidence level: 7.98e-01

Nearest Neighbors from the Training Set

Image not found

4-Methylcatechol Measured: 1.37 Predicted: 1.12 Image not found

Paroxypropione Measured: 2.03 Predicted: 1.47 Image not found

Caffeic acid
Measured: 1.15
Predicted: 1.07

Image not found

Ethanone, 1-(3-hydroxyphenyl)-

Measured: 1.39 Predicted: 1.44 Image not found

4-Hydroxyacetophenone

Measured: 1.35 Predicted: 1.44